

Hermitian Tensor Product Approximation of Complex Matrices and Separability

Shao-Ming Fei^{a,b}, Naihuan Jing^{c,d}, Bao-Zhi Sun^a

^a Department of Mathematics, Capital Normal University, Beijing 100037

^b Max-Planck-Institute for Mathematics in the Sciences, 04103 Leipzig

^c Department of Mathematics, North Carolina State University,
Raleigh, NC 27695

^d Department of Mathematics, Hubei University, Wuhan, Hubei 430062

Abstract

The approximation of matrices to the sum of tensor products of Hermitian matrices is studied. A minimum decomposition of matrices on tensor space $H_1 \otimes H_2$ in terms of the sum of tensor products of Hermitian matrices on H_1 and H_2 is presented. From this construction the separability of quantum states is discussed.

PACS numbers: 03.67.-a, 03.65.Ud, 03.65.Ta

MSC numbers:

Key words: Separability; Matrix; Tensor product decomposition

1 Introduction

The quantum entangled states have become one of the key resources in quantum information processing. The study of quantum teleportation, quantum cryptography, quantum dense coding, quantum error correction and parallel computation [1, 2, 3] has spurred a flurry of activities in the investigation of quantum entanglements. Despite the potential applications of quantum entangled states, the theory of quantum entanglement itself is far from being satisfied. The separability for bipartite and multipartite quantum mixed states is one of the important problems in quantum entanglement.

Let H_1 (resp. H_2) be an m (resp. n)-dimensional complex Hilbert space, with $|i\rangle$, $i = 1, \dots, m$ (resp. $|j\rangle$, $j = 1, \dots, n$), as an orthonormal basis. A bipartite mixed state is said to be separable if the density matrix can be written as

$$\rho = \sum_i p_i \rho_i^1 \otimes \rho_i^2, \quad (1)$$

where $0 < p_i \leq 1$, $\sum_i p_i = 1$, ρ_i^1 and ρ_i^2 are rank one density matrices on H_1 and H_2 respectively. It is a challenge to find a decomposition like (1) or proving that it does not exist for a generic mixed state ρ [4, 5, 6]. With considerable effort in analyzing the separability, there have been some (necessary) criteria for separability in recent years, for instance, the Bell inequalities [7], PPT (positive partial transposition)[8] (which is also sufficient for the cases 2×2 and 2×3 bipartite systems [9]), reduction criterion[10, 11], majorization criterion[12], entanglement witnesses [9] and [13, 14], realignment [15, 16, 17] and generalized realignment [18], as well as some necessary and sufficient criteria for low rank density matrices [19, 20, 21] and also for general ones but not operational [9].

In [22] the minimum distance (in the sense of matrix norm) between a given matrix and some other matrices with certain rank is studied. In [23] and [24], for a given matrix A , the minimum of the Frobenius norm like $\|A - \sum_i B_i \otimes C_i\|_F$ is investigated. In this paper we develop the method of Hermitian tensor product approximation for general complex matrix A , i.e. we require B_i and C_i to be Hermitian matrices. By dealing with the Hermitian condition as higher dimensional real constraints, an explicit construction of general matrices on $H_1 \otimes H_2$ according to the sum of the tensor products of Hermitian matrices as well as real symmetric matrices on $H_1 \otimes H_2$ is presented. The results are generalized to the multipartite case. The separability problem is discussed in terms of these tensor product expressions.

2 Tensor product decomposition in terms of real symmetric matrices

We first consider the tensor product decompositions according to real symmetric matrices. Let A be a given $mn \times mn$ real matrix on $H_1 \otimes H_2$. We consider the problem of approximation of A such that the Frobenius norm

$$\|A - \sum_i^r B_i \otimes C_i\|_F \quad (2)$$

is minimized for some $m \times m$ real symmetric matrix B_i on H_1 and $n \times n$ real symmetric matrix C_i on H_2 , $i = 1, \dots, r \in \mathbb{N}$.

We first introduce some notations. For an $m \times m$ block matrix Z with each block Z_{ij} of size $n \times n$, $i, j = 1, \dots, m$, the realigned matrix \tilde{Z} is defined by

$$\tilde{Z} = [\text{vec}(Z_{11}), \dots, \text{vec}(Z_{m1}), \dots, \text{vec}(Z_{1m}), \dots, \text{vec}(Z_{mm})]^t,$$

where for any $m \times n$ matrix T with entries t_{ij} , $\text{vec}(T)$ is defined to be

$$\text{vec}(T) = [t_{11}, \dots, t_{m1}, t_{12}, \dots, t_{m2}, \dots, t_{1n}, \dots, t_{mn}]^t.$$

There is also another useful definition of \tilde{Z} , $(\tilde{Z})_{ij,kl} = (Z)_{ik,jl}$. A matrix Z can be expressed as the tensor product of two matrices V_1 on H_1 and V_2 on H_2 , $Z = V_1 \otimes V_2$ if and only if (cf, e.g., [24]) $\tilde{Z} = \text{vec}(V_1)\text{vec}(V_2)^t$, i.e., the rank of \tilde{Z} is one, $r(\tilde{Z}) = 1$.

Due to the property of the Frobenius norm, we have

$$\|A - \sum_{i=1}^r B_i \otimes C_i\|_F = \|\tilde{A} - \sum_{i=1}^r \text{vec}(B_i)\text{vec}(C_i)^t\|_F. \quad (3)$$

The symmetric condition of the matrices B_i and C_i can be expressed in terms of some real matrices S_1 and S_2 in a form

$$S_1^t \text{vec}(B_i) = S_2^t \text{vec}(C_i) = 0, \quad i = 1, \dots, r. \quad (4)$$

We define Q_s to be an $m^2 \times \frac{m(m-1)}{2}$ matrix such that, if we arrange the row indices of Q_s as $\{11, 21, 31, \dots, m1, 12, 22, 32, \dots, m2, \dots, mm\}$, then all the entries of Q_s are zero except those at 21 and 12 (resp. 31 and 13, ...) which are 1 and -1 respectively in the first (resp. second, ...) column. We simply denote

$$Q_s = [\{e_{21}, -e_{12}\}; \{e_{31}, -e_{13}\}; \dots; \{e_{m,m-1}, -e_{m-1,m}\}], \quad (5)$$

where $\{e_{21}, -e_{12}\}$ is first column of Q_s , with 1 and -1 at the 21 and 12 rows respectively; while $\{e_{31}, -e_{13}\}$ is second column of Q_s , with 1 and -1 at the 31 and 13 rows respectively; and so on.

Similarly we define Q_a to be an $m^2 \times \frac{m(m+1)}{2}$ matrix such that

$$Q_a = [\{e_{11}\}; \{e_{21}, e_{12}\}; \{e_{31}, e_{13}\}; \dots; \{e_{22}\}; \{e_{32}, e_{23}\}; \{e_{42}, e_{24}\}; \dots; \{e_{m,m-1}, e_{m-1,m}\}, \{e_{mm}\}]. \quad (6)$$

For $m = 2$, we have

$$Q_s = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \quad Q_a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

S_1 can then be expressed as, something like QR decomposition,

$$S_1 = Q_s \equiv Q_1 \begin{pmatrix} R_1 \\ 0 \end{pmatrix}, \quad (7)$$

where R_1 is a full rank $\frac{m(m-1)}{2} \times \frac{m(m-1)}{2}$ matrix, Q_1 is an orthogonal matrix, $Q_1 = (\bar{Q}_s \bar{Q}_a)$, where \bar{Q}_s and \bar{Q}_a are obtained by normalizing the norm of every column vector of Q_s and Q_a to be one.

For the case $m = 2$,

$$Q_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad R_1 = (\sqrt{2}). \quad (8)$$

S_2 has a similar QR decomposition with $S_2 = Q_2 \begin{pmatrix} R_2 \\ 0 \end{pmatrix}$, by replacing the dimension m with n in (7).

Set

$$Q_1^t \tilde{A} Q_2 = \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{A}_{22} \end{pmatrix}. \quad (9)$$

Suppose the singular value decomposition of \hat{A}_{22} is given by $\hat{A}_{22} = \sum_{i=1}^r \sqrt{\lambda_i} u_i v_i^t$, where r and λ_i , $i = 1, 2, \dots, r$, are the rank and eigenvalues of $\hat{A}_{22}^\dagger \hat{A}_{22}$ respectively and u_i (resp. v_i) are the eigenvectors of the matrix $\hat{A}_{22} \hat{A}_{22}^\dagger$ (resp. $\hat{A}_{22}^\dagger \hat{A}_{22}$). Set $\hat{\mathcal{B}}_i = \sqrt{\lambda_i} u_i$, $\hat{\mathcal{C}}_i = v_i$.

[Theorem 1]. Let A be an $mn \times mn$ real matrix on $H_1 \otimes H_2$, where $\dim(H_1) = m$, $\dim(H_2) = n$. The minimum of the Frobenius norm $\|A - \sum_i^r B_i \otimes C_i\|_F$ is obtained for some $m \times m$ real symmetric matrix B_i on H_1 and $n \times n$ real symmetric matrix C_i on H_2 , given by

$$\text{vec}(B_i) = Q_1 \begin{pmatrix} 0 \\ \hat{\mathcal{B}}_i \end{pmatrix}, \quad \text{vec}(C_i) = Q_2 \begin{pmatrix} 0 \\ \hat{\mathcal{C}}_i \end{pmatrix}. \quad (10)$$

[Proof]. Set

$$Q_1^t \text{vec}(B_i) = \begin{pmatrix} \hat{\mathcal{B}}_i \\ \hat{\mathcal{B}}_i \end{pmatrix}, \quad Q_2^t \text{vec}(C_i) = \begin{pmatrix} \hat{\mathcal{C}}_i \\ \hat{\mathcal{C}}_i \end{pmatrix}. \quad (11)$$

From (4) and (7) we have

$$\begin{pmatrix} R_1^t & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathcal{B}}_i \\ \hat{\mathcal{B}}_i \end{pmatrix} = 0, \quad \begin{pmatrix} R_2^t & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathcal{C}}_i \\ \hat{\mathcal{C}}_i \end{pmatrix} = 0,$$

which give rise to $\hat{\mathcal{B}}_i = \hat{\mathcal{C}}_i = 0$, due to the nonsingularity of R_1^t and R_2^t .

From (3), (9) and (11) we obtain

$$\begin{aligned} \|A - \sum_{i=1}^r B_i \otimes C_i\|_F &= \|Q_1^t \tilde{A} Q_2 - \sum_{i=1}^r Q_1^t \text{vec}(B_i) \text{vec}(C_i)^t Q_2\|_F \\ &= \left\| \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{A}_{22} \end{pmatrix} - \sum_{i=1}^r \begin{pmatrix} 0 \\ \hat{\mathcal{B}}_i \end{pmatrix} \begin{pmatrix} 0 & \hat{\mathcal{C}}_i^t \end{pmatrix} \right\|_F \\ &= \left\| \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{A}_{22} \end{pmatrix} - \sum_{i=1}^r \begin{pmatrix} 0 & 0 \\ 0 & \hat{\mathcal{B}}_i \hat{\mathcal{C}}_i^t \end{pmatrix} \right\|_F \\ &= \sqrt{\|\hat{A}_{11}\|_F^2 + \|\hat{A}_{12}\|_F^2 + \|\hat{A}_{21}\|_F^2 + \|\hat{A}_{22} - \sum_{i=1}^r \hat{\mathcal{B}}_i \hat{\mathcal{C}}_i^t\|_F^2}. \end{aligned}$$

From matrix approximation we have that $\hat{A}_{22} = \sum_{i=1}^r \hat{\mathcal{B}}_i \hat{\mathcal{C}}_i^t$ is the singular value decomposition (SVD) for \hat{A}_{22} , which results in formula (10). \square .

From Theorem 1 we see that if a real symmetric matrix A has a decomposition of tensor product of real symmetric matrices, then $\hat{A}_{11} = \hat{A}_{12} = \hat{A}_{21} = 0$. As an example we consider the Werner state [25],

$$\rho_w = \frac{1-F}{3} I_{4 \times 4} + \frac{4F-1}{3} |\Psi^-\rangle \langle \Psi^-| = \begin{pmatrix} \frac{1-F}{3} & 0 & 0 & 0 \\ 0 & \frac{2F+1}{6} & \frac{1-4F}{6} & 0 \\ 0 & \frac{1-4F}{6} & \frac{2F+1}{6} & 0 \\ 0 & 0 & 0 & \frac{1-F}{3} \end{pmatrix}, \quad (12)$$

where $|\Psi^-\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$. State ρ_w is separable for $F \leq 1/2$ and entangled for

$1/2 < F \leq 1$. According to the definition of realignment we have

$$\tilde{\rho}_w = \begin{pmatrix} \frac{1-F}{3} & 0 & 0 & \frac{2F+1}{6} \\ 0 & 0 & \frac{1-4F}{6} & 0 \\ 0 & \frac{1-4F}{6} & 0 & 0 \\ \frac{2F+1}{6} & 0 & 0 & \frac{1-F}{3} \end{pmatrix}.$$

Here the dimension $m = n$, hence $Q_2 = Q_1$ is given by (8). From (9) we have

$$Q_1^t \tilde{\rho}_w Q_1 = \begin{pmatrix} \hat{\rho}_{w11} & \hat{\rho}_{w12} \\ \hat{\rho}_{w21} & \hat{\rho}_{w22} \end{pmatrix} = \begin{pmatrix} \frac{4F-1}{6} & 0 & 0 & 0 \\ 0 & \frac{1-F}{3} & 0 & \frac{2F+1}{6} \\ 0 & 0 & \frac{1-4F}{6} & 0 \\ 0 & \frac{2F+1}{6} & 0 & \frac{1-F}{3} \end{pmatrix}.$$

Therefore ρ_w is generally not decomposable according to real symmetric matrices because $(\hat{\rho}_w)_{11} = (4F - 1)/6 \neq 0$ as long as $F \neq 1/4$. From the singular value decomposition of $(\hat{\rho}_w)_{22}$,

$$(\hat{\rho}_w)_{22} = \begin{pmatrix} \frac{1-F}{3} & 0 & \frac{2F+1}{6} \\ 0 & \frac{1-4F}{6} & 0 \\ \frac{2F+1}{6} & 0 & \frac{1-F}{3} \end{pmatrix}$$

we have:

$$u_1 = v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \varepsilon u_2 = v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \quad \varepsilon u_3 = v_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

with eigenvalues $\lambda_1 = 1/4$, $\lambda_2 = \lambda_3 = (1-4F)^2/36$ respectively, where $\varepsilon = (1-4F)/|1-4F|$. From (10) we have $\text{vec}(B_1) = \sqrt{\lambda_1}(1/\sqrt{2}, 0, 0, 1/\sqrt{2})^t$, $\text{vec}(B_2) = \varepsilon\sqrt{\lambda_2}(-1/\sqrt{2}, 0, 0, 1/\sqrt{2})^t$, $\text{vec}(B_3) = \varepsilon\sqrt{\lambda_3}(0, 1/\sqrt{2}, 1/\sqrt{2}, 0)^t$. Therefore the best real symmetric matrix tensor product decomposition is

$$\rho_w \approx \frac{1}{4} I_{2 \times 2} \otimes I_{2 \times 2} + \frac{1-4F}{12} (\sigma_1 \otimes \sigma_1 + \sigma_3 \otimes \sigma_3),$$

where σ_i are Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

3 Hermitian tensor product decomposition of Hermitian matrices

We consider now the tensor product decompositions according to Hermitian matrices. Let A be a given $mn \times mn$ complex matrix on $H_1 \otimes H_2$. We first consider the problem of approximation of A such that the Frobenius norm

$$\|A - B \otimes C\|_F = \|\tilde{A} - \text{vec}(B)\text{vec}(C)^t\|_F. \quad (13)$$

is minimized for some $m \times m$ Hermitian matrix B on H_1 and $n \times n$ Hermitian matrix C on H_2 .

In order to impose the Hermitian condition of the matrices B and C , we separate the matrices B and C into real and imaginary parts such that $B = \mathbf{B} + i\mathcal{B}$, $C = \mathbf{C} + i\mathcal{C}$, where \mathbf{B} and \mathbf{C} (resp. \mathcal{B} and \mathcal{C}) are the real (resp. imaginary) parts of B and C respectively. As $\text{vec}(B) = \text{vec}(\mathbf{B}) + i \text{vec}(\mathcal{B})$, we have

$$\text{vec}(B)\text{vec}(C)^t = (\text{vec}(\mathbf{B})\text{vec}(\mathbf{C})^t - \text{vec}(\mathcal{B})\text{vec}(\mathcal{C})^t) + i(\text{vec}(\mathbf{B})\text{vec}(\mathcal{C})^t + \text{vec}(\mathcal{B})\text{vec}(\mathbf{C})^t).$$

We now map the complex matrix A to be a real one:

$$A \longrightarrow \begin{pmatrix} \mathbf{A} & \mathcal{A} \\ -\mathcal{A} & \mathbf{A} \end{pmatrix},$$

where \mathbf{A} and \mathcal{A} are the real and the imaginary parts of A respectively. Now the approximation problem of complex matrices to the tensor product of two Hermitian matrices is reduced to the problem of real matrices and the results in [23, 24] can be used accordingly. The problem to minimize $\|\tilde{A} - \text{vec}(B)\text{vec}(C)^t\|_F$ is reduced to minimize

$$\left\| \begin{pmatrix} \tilde{\mathbf{A}} & \tilde{\mathcal{A}} \\ -\tilde{\mathcal{A}} & \tilde{\mathbf{A}} \end{pmatrix} - \begin{pmatrix} \text{vec}(\mathbf{B}) & \text{vec}(\mathcal{B}) \\ -\text{vec}(\mathcal{B}) & \text{vec}(\mathbf{B}) \end{pmatrix} \begin{pmatrix} \text{vec}(\mathbf{C}) & -\text{vec}(\mathcal{C}) \\ \text{vec}(\mathcal{C}) & \text{vec}(\mathbf{C}) \end{pmatrix}^t \right\|_F \quad (14)$$

under the Hermitian condition: $B = B^\dagger$, $C = C^\dagger$, i.e., \mathbf{B} and \mathbf{C} are symmetric, \mathcal{B} and \mathcal{C} are antisymmetric. This condition can be expressed in terms of some real matrices S_1 and S_2 in a form

$$S_1^t \begin{pmatrix} \text{vec}(\mathbf{B}) \\ \pm \text{vec}(\mathcal{B}) \end{pmatrix} = S_2^t \begin{pmatrix} \text{vec}(\mathbf{C}) \\ \pm \text{vec}(\mathcal{C}) \end{pmatrix} = 0. \quad (15)$$

[Lemma 1]. Condition (15) has a QR decomposition such that

$$S_1 = Q_1 \begin{pmatrix} R_1 \\ 0 \end{pmatrix}, \quad S_2 = Q_2 \begin{pmatrix} R_2 \\ 0 \end{pmatrix}, \quad (16)$$

where R_1 and R_2 are full rank matrices, Q_1 and Q_2 are orthogonal matrices.

[Proof]. S_1 can be generally expressed as

$$S_1 = \begin{pmatrix} Q_s & 0 \\ 0 & Q_a \end{pmatrix},$$

where Q_s and Q_a are given by (5) and (6) respectively. The QR decomposition of S_1 is given by

$$Q_1 = \begin{pmatrix} \bar{Q}_s & 0 & 0 & \bar{Q}_a \\ 0 & \bar{Q}_a & \bar{Q}_s & 0 \end{pmatrix} \equiv \begin{pmatrix} X_1 & Y_1 \\ Y_1 & X_1 \end{pmatrix}, \quad (17)$$

with \bar{Q}_s and \bar{Q}_a given in section 2, X_1 (resp. Y_1) is an $m^2 \times m^2$ matrix with the first $m(m-1)/2$ (resp. last $m(m+1)/2$) columns replaced by the matrix \bar{Q}_s (resp. \bar{Q}_a) and the rest entries zero, R_1 is a diagonal matrix with diagonal elements either 1 or $\sqrt{2}$. For the case $m = 2$,

$$X_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad Y_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad R_1 = \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (18)$$

S_2 has a similar QR decomposition with

$$Q_2 = \begin{pmatrix} X_2 & Y_2 \\ Y_2 & X_2 \end{pmatrix}, \quad (19)$$

by replacing the dimension m with n in the expression of S_1 . \square

Set

$$\begin{aligned} Q_1^t \begin{pmatrix} \text{vec}(\mathbf{B}) \\ -\text{vec}(\mathcal{B}) \end{pmatrix} &\equiv \begin{pmatrix} \hat{\mathbf{B}} \\ -\hat{\mathcal{B}} \end{pmatrix}, & Q_1^t \begin{pmatrix} \text{vec}(\mathbf{B}) \\ \text{vec}(\mathcal{B}) \end{pmatrix} &\equiv \begin{pmatrix} \check{\mathbf{B}} \\ \check{\mathcal{B}} \end{pmatrix}, \\ Q_2^t \begin{pmatrix} \text{vec}(\mathbf{C}) \\ -\text{vec}(\mathcal{C}) \end{pmatrix} &\equiv \begin{pmatrix} \hat{\mathbf{C}} \\ -\hat{\mathcal{C}} \end{pmatrix}, & Q_2^t \begin{pmatrix} \text{vec}(\mathbf{C}) \\ \text{vec}(\mathcal{C}) \end{pmatrix} &\equiv \begin{pmatrix} \check{\mathbf{C}} \\ \check{\mathcal{C}} \end{pmatrix}. \end{aligned} \quad (20)$$

From (15) and (16) we have

$$\begin{aligned} \begin{pmatrix} R_1^t & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{B}} \\ -\hat{\mathcal{B}} \end{pmatrix} &= 0, & \begin{pmatrix} R_1^t & 0 \end{pmatrix} \begin{pmatrix} \check{\mathbf{B}} \\ \check{\mathcal{B}} \end{pmatrix} &= 0, \\ \begin{pmatrix} R_2^t & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{C}} \\ -\hat{\mathcal{C}} \end{pmatrix} &= 0, & \begin{pmatrix} R_2^t & 0 \end{pmatrix} \begin{pmatrix} \check{\mathbf{C}} \\ \check{\mathcal{C}} \end{pmatrix} &= 0, \end{aligned}$$

which give rise to $\hat{\mathbf{B}} = \check{\mathbf{B}} = \hat{\mathbf{C}} = \check{\mathbf{C}} = 0$, due to the nonsingularity of R_1^t and R_2^t .

Therefore we have

$$\begin{aligned} \begin{pmatrix} \text{vec}(\mathbf{B}) \\ -\text{vec}(\mathcal{B}) \end{pmatrix} &= Q_1 \begin{pmatrix} \hat{\mathbf{B}} \\ -\hat{\mathcal{B}} \end{pmatrix} = \begin{pmatrix} X_1 & Y_1 \\ Y_1 & X_1 \end{pmatrix} \begin{pmatrix} 0 \\ -\hat{\mathcal{B}} \end{pmatrix} = \begin{pmatrix} -Y_1 \hat{\mathcal{B}} \\ -X_1 \hat{\mathcal{B}} \end{pmatrix}, \\ \begin{pmatrix} \text{vec}(\mathbf{B}) \\ \text{vec}(\mathcal{B}) \end{pmatrix} &= Q_1 \begin{pmatrix} \check{\mathbf{B}} \\ \check{\mathcal{B}} \end{pmatrix} = \begin{pmatrix} X_1 & Y_1 \\ Y_1 & X_1 \end{pmatrix} \begin{pmatrix} 0 \\ \check{\mathcal{B}} \end{pmatrix} = \begin{pmatrix} Y_1 \check{\mathcal{B}} \\ X_1 \check{\mathcal{B}} \end{pmatrix}. \end{aligned} \quad (21)$$

Thus $-Y_1 \hat{\mathcal{B}} = Y_1 \check{\mathcal{B}}$, $X_1 \hat{\mathcal{B}} = X_1 \check{\mathcal{B}}$ and

$$\check{\mathcal{B}} = (X_1 + Y_1)^{-1}(X_1 - Y_1)\hat{\mathcal{B}} = \begin{pmatrix} \bar{Q}_s^t \\ \bar{Q}_a^t \end{pmatrix} \begin{pmatrix} \bar{Q}_s & -\bar{Q}_a \end{pmatrix} \hat{\mathcal{B}} = I_{s,a}^m \hat{\mathcal{B}}, \quad (22)$$

where $I_{s,a}^m = \text{diag}(I_s^m, -I_a^m)$, I_s^m (resp. I_a^m) is an $m(m-1)/2$ (resp. $m(m+1)/2$) dimensional identity matrix.

Let P denote the permutation matrix,

$$P = \begin{pmatrix} 0 & I_{m^2 \times m^2} \\ I_{m^2 \times m^2} & 0 \end{pmatrix}.$$

It is easily seen that $PQ_1P = Q_1$. From the second formula in (21) we have

$$Q_1^t \begin{pmatrix} \text{vec}(\mathcal{B}) \\ \text{vec}(\mathbf{B}) \end{pmatrix} = \begin{pmatrix} \check{\mathcal{B}} \\ 0 \end{pmatrix}.$$

Hence we have

$$Q_1^t \begin{pmatrix} \text{vec}(\mathbf{B}) & \text{vec}(\mathcal{B}) \\ -\text{vec}(\mathcal{B}) & \text{vec}(\mathbf{B}) \end{pmatrix} = \begin{pmatrix} 0 & \check{\mathcal{B}} \\ -\hat{\mathcal{B}} & 0 \end{pmatrix}, \quad (23)$$

and, similarly,

$$Q_2^t \begin{pmatrix} \text{vec}(\mathcal{C}) & -\text{vec}(\mathcal{C}) \\ \text{vec}(\mathcal{C}) & \text{vec}(\mathcal{C}) \end{pmatrix} = \begin{pmatrix} 0 & -\hat{\mathcal{C}} \\ \check{\mathcal{C}} & 0 \end{pmatrix}, \quad (24)$$

where

$$\check{\mathcal{C}} = I_{s,a}^n \hat{\mathcal{C}}, \quad (25)$$

$I_{s,a}^n = \text{diag}(I_s^n, -I_a^n)$, I_s^n (resp. I_a^n) is an $n(n-1)/2$ (resp. $n(n+1)/2$) dimensional identity matrix.

Set

$$Q_1^t \begin{pmatrix} \tilde{\mathbf{A}} & \tilde{\mathcal{A}} \\ -\tilde{\mathcal{A}} & \tilde{\mathbf{A}} \end{pmatrix} Q_2 \equiv \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{A}_{22} \end{pmatrix}. \quad (26)$$

That is

$$\begin{aligned} \hat{A}_{11} &= X_1^t \tilde{\mathbf{A}} X_2 + Y_1^t \tilde{\mathbf{A}} Y_2 + X_1^t \tilde{\mathcal{A}} Y_2 - Y_1^t \tilde{\mathcal{A}} X_2, \\ \hat{A}_{12} &= X_1^t \tilde{\mathbf{A}} Y_2 + Y_1^t \tilde{\mathbf{A}} X_2 + X_1^t \tilde{\mathcal{A}} X_2 - Y_1^t \tilde{\mathcal{A}} Y_2, \\ \hat{A}_{21} &= Y_1^t \tilde{\mathbf{A}} X_2 + X_1^t \tilde{\mathbf{A}} Y_2 + Y_1^t \tilde{\mathcal{A}} Y_2 - X_1^t \tilde{\mathcal{A}} X_2, \\ \hat{A}_{22} &= Y_1^t \tilde{\mathbf{A}} Y_2 + X_1^t \tilde{\mathbf{A}} X_2 + Y_1^t \tilde{\mathcal{A}} X_2 - X_1^t \tilde{\mathcal{A}} Y_2. \end{aligned}$$

[Theorem 2]. To minimize (13) is equivalent to minimize the following formula

$$\sqrt{\|\hat{A}_{22} + \check{\mathcal{B}}\check{\mathcal{C}}^t\|_F^2 + \|\hat{A}_{11} + \check{\mathcal{B}}\hat{\mathcal{C}}^t\|_F^2 + \|\hat{A}_{12}\|_F^2 + \|\hat{A}_{21}\|_F^2}. \quad (27)$$

[Proof]. From (14), (23) and (24) we obtain

$$\begin{aligned} & \left\| \begin{pmatrix} \tilde{\mathbf{A}} & \tilde{\mathcal{A}} \\ -\tilde{\mathcal{A}} & \tilde{\mathbf{A}} \end{pmatrix} - \begin{pmatrix} \text{vec}(\mathbf{B}) & \text{vec}(\mathcal{B}) \\ -\text{vec}(\mathcal{B}) & \text{vec}(\mathbf{B}) \end{pmatrix} \begin{pmatrix} \text{vec}(\mathcal{C}) & -\text{vec}(\mathcal{C}) \\ \text{vec}(\mathcal{C}) & \text{vec}(\mathcal{C}) \end{pmatrix}^t \right\|_F \\ &= \left\| Q_1^t \begin{pmatrix} \tilde{\mathbf{A}} & \tilde{\mathcal{A}} \\ -\tilde{\mathcal{A}} & \tilde{\mathbf{A}} \end{pmatrix} Q_2 - Q_1^t \begin{pmatrix} \text{vec}(\mathbf{B}) & \text{vec}(\mathcal{B}) \\ -\text{vec}(\mathcal{B}) & \text{vec}(\mathbf{B}) \end{pmatrix} \begin{pmatrix} \text{vec}(\mathcal{C}) & -\text{vec}(\mathcal{C}) \\ \text{vec}(\mathcal{C}) & \text{vec}(\mathcal{C}) \end{pmatrix}^t Q_2 \right\|_F \\ &= \left\| \begin{pmatrix} \hat{A}_{11} & \hat{A}_{12} \\ -\hat{A}_{21} & \hat{A}_{22} \end{pmatrix} - \begin{pmatrix} 0 & \check{\mathcal{B}} \\ -\check{\mathcal{B}} & 0 \end{pmatrix} \begin{pmatrix} 0 & -\hat{\mathcal{C}} \\ \check{\mathcal{C}} & 0 \end{pmatrix}^t \right\|_F \\ &= \left\| \begin{pmatrix} \hat{A}_{11} & \hat{A}_{21} \\ -\hat{A}_{21} & \hat{A}_{22} \end{pmatrix} - \begin{pmatrix} -\check{\mathcal{B}}\hat{\mathcal{C}}^t & 0 \\ 0 & -\check{\mathcal{B}}\check{\mathcal{C}}^t \end{pmatrix} \right\|_F \\ &= \sqrt{\|\hat{A}_{22} + \check{\mathcal{B}}\check{\mathcal{C}}^t\|_F^2 + \|\hat{A}_{11} + \check{\mathcal{B}}\hat{\mathcal{C}}^t\|_F^2 + \|\hat{A}_{12}\|_F^2 + \|\hat{A}_{21}\|_F^2}. \end{aligned}$$

□

[Lemma 2]. If the matrix $A = \mathbf{A} + i\mathcal{A}$ is Hermitian, we have the relations:

$$\hat{A}_{12} = \hat{A}_{21} = 0, \quad \hat{A}_{11} = I_{s,a}^m \hat{A}_{22} I_{s,a}^m.$$

[Proof]. As the matrix $A = \mathbf{A} + i\mathcal{A}$ is Hermitian, i.e., \mathbf{A} is symmetric and \mathcal{A} is antisymmetric, we have

$$(\tilde{\mathbf{A}})_{ij,kl} = (\mathbf{A})_{ik,jl} = (\mathbf{A})_{jl,ik} = (\tilde{\mathbf{A}})_{ji,lk}, \quad (\tilde{\mathcal{A}})_{ij,kl} = (\mathcal{A})_{ik,jl} = -(\mathcal{A})_{jl,ik} = -(\tilde{\mathcal{A}})_{ji,lk}.$$

Noting that in our construction of X_α and Y_α , $(X_\alpha)_{ij,kl} = -(X_\alpha)_{ji,kl}$, $(Y_\alpha)_{ij,kl} = (Y_\alpha)_{ji,kl}$, $\alpha = 1, 2$, we obtain

$$(X_1^t \tilde{A} Y_2)_{ij,pq} = (X_1)_{kl,ij} (\tilde{A})_{kl,mn} (Y_2)_{mn,pq} = -(X_1^t \tilde{A} Y_2)_{ij,pq} = 0.$$

Similarly we have $Y_1^t \tilde{A} X_2 = X_1^t \tilde{A} X_2 = Y_1^t \tilde{A} Y_2 = 0$. Hence $\hat{A}_{12} = \hat{A}_{21} = 0$.

From the relations $I_{s,a}^m Y_1 = -Y_1$, $I_{s,a}^m X_1 = X_1$ and $Y_2 I_{s,a}^n = -Y_2$, $I_{s,a}^n X_2 = X_2$, we have $I_{s,a}^m (Y_1^t \tilde{A} Y_2 + X_1^t \tilde{A} X_2) I_{s,a}^n = Y_1^t \tilde{A} Y_2 + X_1^t \tilde{A} X_2$ and $I_{s,a}^m (Y_1^t \tilde{A} X_2 - X_1^t \tilde{A} Y_2) I_{s,a}^n = -(Y_1^t \tilde{A} X_2 - X_1^t \tilde{A} Y_2)$. Therefore $\hat{A}_{11} = I_{s,a}^m \hat{A}_{22} I_{s,a}^n$ or $\hat{A}_{22} = I_{s,a}^m \hat{A}_{11} I_{s,a}^n$. \square

For Hermitian matrix A , by using (22), (25) and Lemma 2 we have $\|\hat{A}_{11} + \check{\mathcal{B}}\check{\mathcal{C}}^t\|_F = \|\hat{A}_{11} + I_{s,a}^m \check{\mathcal{B}}\check{\mathcal{C}}^t I_{s,a}^n\|_F = \|I_{s,a}^m \hat{A}_{11} I_{s,a}^n + \check{\mathcal{B}}\check{\mathcal{C}}^t\|_F = \|\hat{A}_{22} + \check{\mathcal{B}}\check{\mathcal{C}}^t\|_F$. From Lemma 2 we have that to minimize $\|A - B \otimes C\|_F$ (13) is equivalent to minimize $\|\hat{A}_{22} + \check{\mathcal{B}}\check{\mathcal{C}}^t\|_F$, which maybe zero, when $\hat{A}_{22} = -\check{\mathcal{B}}\check{\mathcal{C}}^t$.

Now the minimum of the Frobenius norm $\|A - \sum_i^r B_i \otimes C_i\|_F$ can be obtained readily. Suppose the singular value decomposition of \hat{A}_{22} is $\hat{A}_{22} = \sum_{i=1}^r \sqrt{\lambda_i} u_i v_i^t$, where r and λ_i , $i = 1, 2, \dots, r$, are the rank and eigenvalues of $\hat{A}_{22}^\dagger \hat{A}_{22}$ respectively and u_i (resp. v_i) are the eigenvectors of the matrix $\hat{A}_{22} \hat{A}_{22}^\dagger$ (resp. $\hat{A}_{22}^\dagger \hat{A}_{22}$). Set $\hat{\mathcal{B}}_i = \sqrt{\lambda_i} u_i$, $\check{\mathcal{C}}_i = -v_i$. By using the results in [23, 24], for Hermitian matrix A the minimum of $\|A - \sum_{i=1}^r B_i \otimes C_i\|_F$ is obtained when $\hat{A}_{22} = -\sum_{i=1}^r \hat{\mathcal{B}}_i \check{\mathcal{C}}_i^t$.

[Theorem 3]. Let A be an $mn \times mn$ Hermitian matrix on $H_1 \otimes H_2$, where $\dim(H_1) = m$, $\dim(H_2) = n$. The minimum of the Frobenius norm $\|A - \sum_i^r B_i \otimes C_i\|_F$ is obtained for some $m \times m$ Hermitian matrix B on H_1 and $n \times n$ Hermitian matrix C on H_2 , if $\hat{A}_{22} = -\sum_{i=1}^r \hat{\mathcal{B}}_i \check{\mathcal{C}}_i^t$, where \hat{A}_{22} is defined by (26), $B_i = \mathcal{B}_i + i\mathcal{B}_i$, $C_i = \mathcal{C}_i + i\mathcal{C}_i$, are given by the relations

$$\begin{pmatrix} \text{vec}(\mathcal{B}_i) \\ -\text{vec}(\mathcal{B}_i) \end{pmatrix} = Q_1 \begin{pmatrix} 0 \\ -\hat{\mathcal{B}}_i \end{pmatrix}, \quad \begin{pmatrix} \text{vec}(\mathcal{C}_i) \\ \text{vec}(\mathcal{C}_i) \end{pmatrix} = Q_2 \begin{pmatrix} 0 \\ \check{\mathcal{C}}_i \end{pmatrix}. \quad (28)$$

As an example we consider the bound entangled state on 2×4 ($m = 2$, $n = 4$) [26],

$$\rho_b = \frac{1}{7b+1} \begin{pmatrix} b & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & b & 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & b & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1+b}{2} & 0 & 0 & \frac{\sqrt{1-b^2}}{2} \\ b & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & b & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & b & 0 & \frac{\sqrt{1-b^2}}{2} & 0 & 0 & \frac{1+b}{2} \end{pmatrix}, \quad (29)$$

where $0 < b < 1$. ρ_b is a PPT but entangled state. The QR decomposition in our case only depends the dimensions. Q_1 is still given by (17) and (18). Q_2 is a 32×32 matrix with X_2 , Y_2 in (19) given by $X_2 = (\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3, \mathbf{f}_4, \mathbf{f}_5, \mathbf{f}_6, \mathbf{0}_{10})$, $Y_2 = (\mathbf{0}_6, \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_5, \mathbf{a}_6, \mathbf{a}_7, \mathbf{a}_8, \mathbf{a}_9, \mathbf{a}_{10})$,

where \mathbf{s}_i and \mathbf{a}_i are 16×1 column vectors:

$$\begin{aligned}
\mathbf{f}_1 &= (0, 1/\sqrt{2}, 0, 0, -1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{f}_2 &= (0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, -1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{f}_3 &= (0, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1/\sqrt{2}, 0, 0)^t, \\
\mathbf{f}_4 &= (0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, -1/\sqrt{2}, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{f}_5 &= (0, 0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0, -1/\sqrt{2}, 0)^t, \\
\mathbf{f}_6 &= (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, -1/\sqrt{2}, 0, 0)^t, \\
\mathbf{a}_1 &= (1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{a}_2 &= (0, 1/\sqrt{2}, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{a}_3 &= (0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{a}_4 &= (0, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 0)^t, \\
\mathbf{a}_5 &= (0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{a}_6 &= (0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0)^t, \\
\mathbf{a}_7 &= (0, 0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0)^t, \\
\mathbf{a}_8 &= (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0)^t, \\
\mathbf{a}_9 &= (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 1/\sqrt{2}, 0)^t, \\
\mathbf{a}_{10} &= (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1)^t,
\end{aligned}$$

$\mathbf{0}_6$ and $\mathbf{0}_{10}$ are 16×6 and 16×10 null matrices. From (26) we have

$$Q_1^t \begin{pmatrix} \tilde{\rho}_b & 0 \\ 0 & \tilde{\rho}_b \end{pmatrix} Q_2 \equiv \begin{pmatrix} \hat{A}_{11} & 0 \\ 0 & \hat{A}_{22} \end{pmatrix},$$

where

$$\hat{A}_{11} = \hat{A}_{22} = \frac{1}{1+7b} \begin{pmatrix} b & 0 & 0 & b & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & b & 0 & b \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & b & 0 & 0 & b & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1+b}{2} & 0 & 0 & \sqrt{\frac{1-b^2}{2}} & b & 0 & 0 & b & 0 & \frac{1+b}{2} \end{pmatrix}.$$

From the singular value decomposition of \hat{A}_{11} we have

$$\begin{aligned}
\hat{\mathcal{B}}_1 &= \frac{\sqrt{3}b}{1+7b}(0, 0, 1, 0)^t, & \hat{\mathcal{B}}_3 &= \frac{\sqrt{\lambda_-}}{(1+7b)\sqrt{1+D_+^2}}(0, D_+, 0, 1)^t, \\
\hat{\mathcal{B}}_2 &= \frac{\sqrt{3}b}{1+7b}(1, 0, 0, 0)^t, & \hat{\mathcal{B}}_4 &= \frac{\sqrt{\lambda_+}}{(1+7b)\sqrt{1+D_-^2}}(0, D_-, 0, 1)^t,
\end{aligned}$$

and

$$\begin{aligned}
\check{\mathcal{C}}_1 &= -\frac{1}{\sqrt{3}}(0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 1, 0)^t, \\
\check{\mathcal{C}}_2 &= -\frac{1}{\sqrt{3}}(1, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^t, \\
\check{\mathcal{C}}_3 &= -\frac{1}{\sqrt{\lambda_-(1+D_+^2)}}(0, 0, 0, 0, 0, 0, bD_+ + \frac{1+b}{2}, 0, 0, \sqrt{\frac{1-b^2}{2}}, b(1+D_+), 0, 0, b(1+D_+), 0, bD_+ + \frac{1+b}{2})^t, \\
\check{\mathcal{C}}_4 &= -\frac{1}{\sqrt{\lambda_+(1+D_-^2)}}(0, 0, 0, 0, 0, 0, bD_- + \frac{1+b}{2}, 0, 0, \sqrt{\frac{1-b^2}{2}}, b(1+D_-), 0, 0, b(1+D_-), 0, bD_- + \frac{1+b}{2})^t,
\end{aligned}$$

where

$$\lambda_{\pm} = \frac{1+b+6b^2 \pm \sqrt{1+2b+b^2+20b^3+40b^4}}{2},$$

$$D_{\pm} = -\frac{1+b-2b^2 \pm \sqrt{1+2b+b^2+20b^3+40b^4}}{2b(1+3b)}.$$

Using (28) we have

$$\begin{aligned} \rho_b = & \frac{b}{2(1+7b)} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} + \frac{b}{2(1+7b)} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & i & 0 \\ 0 & -i & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix} \\ & + \frac{1}{(1+7b)(1+D_+^2)} \begin{pmatrix} D_+ & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} \frac{1+b}{2} + bD_+ & 0 & 0 & \frac{1-b^2}{2} \\ 0 & b(1+D_+) & 0 & 0 \\ 0 & 0 & b(1+D_+) & 0 \\ \frac{1-b^2}{2} & 0 & 0 & \frac{1+b}{2} + bD_+ \end{pmatrix} \\ & + \frac{1}{(1+7b)(1+D_-^2)} \begin{pmatrix} D_- & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} \frac{1+b}{2} + bD_- & 0 & 0 & \frac{1-b^2}{2} \\ 0 & b(1+D_-) & 0 & 0 \\ 0 & 0 & b(1+D_-) & 0 \\ \frac{1-b^2}{2} & 0 & 0 & \frac{1+b}{2} + bD_- \end{pmatrix}. \end{aligned} \quad (30)$$

4 Separability of bipartite mixed states

In this section we discuss some properties related to the Hermitian tensor product decomposition that could give rise to some hints to the separability problem of bipartite mixed states. From Theorem 3 we can always calculate the tensor product decomposition in terms of Hermitian matrices for a given density matrix A , $A = \sum_{i=1}^r B_i \otimes C_i$. Nevertheless the Hermitian matrices B_i and C_i are generally not positive. They are not density matrices defined on the subspaces H_1 and H_2 . Hence one can not say that A is separable.

Let $m(A)$ and $M(A)$ denote the smallest and the largest eigenvalues of a Hermitian matrix A . We can transform the decomposition into the one given by another set of Hermitian

matrices which all have the smallest eigenvalue zero, as follows,

$$\begin{aligned}
A &= \sum_{i=1}^r B_i \otimes C_i = \sum_{i=1}^r (B_i - m(B_i)I_m + m(B_i)I_m) \otimes (C_i - m(C_i)I_n + m(C_i)I_n) \\
&= \sum_{i=1}^r (B_i - m(B_i)I_m) \otimes (C_i - m(C_i)I_n) + \sum_{i=1}^r m(C_i)(B_i - m(B_i)I_m) \otimes I_n \\
&\quad + I_m \otimes \sum_{i=1}^r m(B_i)(C_i - m(C_i)I_n) + \sum_{i=1}^r m(B_i)m(C_i)I_m \otimes I_n \\
&= \sum_{i=1}^r (B_i - m(B_i)I_m) \otimes (C_i - m(C_i)I_n) \\
&\quad + \left[\sum_{i=1}^r m(C_i)(B_i - m(B_i)I_m) - m \left(\sum_{i=1}^r m(C_i)(B_i - m(B_i)I_m) \right) I_m \right] \otimes I_n \\
&\quad + I_m \otimes \left[\sum_{i=1}^r m(B_i)(C_i - m(C_i)I_n) - m \left(\sum_{i=1}^r m(B_i)(C_i - m(C_i)I_n) \right) I_n \right] \\
&\quad + \left[m \left(\sum_{i=1}^r m(C_i)B_i \right) + m \left(\sum_{i=1}^r m(B_i)C_i \right) - \sum_{i=1}^r m(B_i)m(C_i) \right] I_m \otimes I_n,
\end{aligned} \tag{31}$$

where I_m and I_n stand for $m \times m$ and $n \times n$ identity matrices. The coefficient of $I_m \otimes I_n$,

$$q_{B,C} \equiv m \left(\sum_{i=1}^r m(C_i)B_i \right) + m \left(\sum_{i=1}^r m(B_i)C_i \right) - \sum_{i=1}^r m(B_i)m(C_i)$$

associated with the decomposition $A = \sum_{i=1}^r B_i \otimes C_i$ is not necessary positive.

$q_{B,C}$ is decomposition dependent. Associated with another decomposition $A = \sum_{i=1}^{r'} B'_i \otimes C'_i$ one would obtain $q_{B',C'} \neq q_{B,C}$. We define the maximum value of $q_{B,C}$ to be the *separability indicator* of A , $S(A) = \max(q_{B,C})$ for all possible Hermitian decompositions of A . With respect to $S(A)$ the associated decomposition is generally of the form

$$A = \sum_i \bar{B}_i \otimes \bar{C}_i + I_m \otimes \bar{C} + \bar{B} \otimes I_n + S(A)I_m \otimes I_n, \tag{32}$$

where $\bar{B}_i \geq 0$, $\bar{C}_i \geq 0$, $\bar{B} \geq 0$, $\bar{C} \geq 0$ are positive Hermitian matrices.

[Theorem 4]. Let A be a Hermitian positive matrix with tensor product decompositions of Hermitian matrices like $A = \sum_{i=1}^r B_i \otimes C_i$. A is separable if and only if the separability indicator $S(A) \geq 0$. Moreover $S(A)$ satisfies the following relations:

$$S(A) \leq m(A), \tag{33}$$

$$\begin{aligned}
S(A) &\geq \frac{1}{2} \sum_{i=1}^r [M(B_i)m(C_i) + M(C_i)m(B_i) \\
&\quad - |m(B_i)|(M(C_i) - m(C_i)) - |m(C_i)|(M(B_i) - m(B_i))],
\end{aligned} \tag{34}$$

$$S(A) \geq m(A) - \sum_i M(\bar{B}_i)M(\bar{C}_i). \tag{35}$$

[Proof]. If A is separable, A has a decomposition $A = \sum_i B_i \otimes C_i$ of the form (1), i.e., $m(B_i) \geq 0$, $m(C_i) \geq 0$. We have

$$\begin{aligned} S(A) \geq q_{B,C} &= m\left(\sum_i m(C_i)B_i\right) + m\left(\sum_i m(B_i)C_i\right) - \sum_i m(B_i)m(C_i) \\ &\geq \sum_i m(C_i)m(B_i) + \sum_i m(B_i)m(C_i) - \sum_i m(B_i)m(C_i) \\ &= \sum_i m(B_i)m(C_i) \geq 0. \end{aligned}$$

If $S(A) \geq 0$, then the associated decomposition (32) is already a separable expression of A .

From the decomposition (32) with respect to $S(A)$, we have

$$m(A) \geq \sum_i m(\bar{B}_i \otimes \bar{C}_i) + m(\bar{B}) + m(\bar{C}) + S(A) = S(A).$$

On the other hand we have

$$\begin{aligned} S(A) &\geq q_{B,C} \geq \sum_i m(m(C_i)B_i) + \sum_i m(m(B_i)C_i) - \sum_i m(B_i)m(C_i) \\ &= \sum_i \left(m(B_i) \frac{m(C_i) + |m(C_i)|}{2} + M(B_i) \frac{m(C_i) - |m(C_i)|}{2} \right) \\ &\quad + \sum_i \left(m(C_i) \frac{m(B_i) + |m(B_i)|}{2} + M(C_i) \frac{m(B_i) - |m(B_i)|}{2} \right) - \sum_i m(B_i)m(C_i), \end{aligned}$$

which is just the formula (34).

By using the relations $M(B + D) \leq M(B) + M(D)$, $m(B + D) \geq m(B) + m(D)$, $m(B + D) \leq m(B) + M(D)$ for any $m \times m$ matrices B and D , we have

$$\begin{aligned} m(A) &= m(\sum_i \bar{B}_i \otimes \bar{C}_i + I_m \otimes \bar{C} + \bar{B} \otimes I_n + S(A)I_m \otimes I_n) \\ &\leq m(I_m \otimes \bar{C} + \bar{B} \otimes I_n + S(A)I_m \otimes I_n) + M(\sum_i \bar{B}_i \otimes \bar{C}_i) \\ &= m(B) + m(C) + S(A) + M(\sum_i \bar{B}_i \otimes \bar{C}_i) \\ &\leq S(A) + \sum_i M(\bar{B}_i)M(\bar{C}_i). \end{aligned}$$

Hence formula (35) follows. \square

Generally $q_{B,C}$ with respect to our decomposition $A = \sum_{i=1}^r B_i \otimes C_i$ does not equal to the separability indicator $S(A)$. Suppose we have another decomposition $A = \sum_{i=1}^{r'} B'_i \otimes C'_i$. As B_i (and C_i) are defined in terms of the singular value decomposition eigenvectors, they are linear independent. We can choose linear functionals φ_i such that $\varphi_i(B_j) = \delta_{ij}$. Applying $\varphi_i \otimes 1$ to both sides of $\sum_{i=1}^r B_i \otimes C_i = \sum_{i=1}^{r'} B'_i \otimes C'_i$ we get $C_i = \sum_{j=1}^{r'} \varphi_i(B'_j)C'_j$, i.e., $C_i \in \langle C'_1, \dots, C'_{r'} \rangle$. Similarly we have $B_i \in \langle B'_1, \dots, B'_{r'} \rangle$. Therefore any other Hermitian decomposition $A = \sum_{i=1}^{r'} B'_i \otimes C'_i$ can be obtained from our decomposition $A = \sum_{i=1}^r B_i \otimes C_i$ in terms of the following transformations

$$B'_j = \sum_{i=1}^r E_{ij}B_i, \quad C'_j = \sum_{i=1}^r F_{ij}C_i,$$

as long as the real matrices $E = (E_{ij})$ and $F = (F_{ij})$ satisfy the relation $EF^t = I_r$.

The inequalities (33)-(35) can be served as separability criterion themselves. For instance, if the minimum eigenvalue of A is zero, then A is entangled if the right hand side of (34) is great than zero.

5 Conclusion and remarks

We have developed a method of Hermitian tensor product approximation of general complex matrices. From which an explicit construction of density matrices on $H_1 \otimes H_2$ in terms of the sum of tensor products of Hermitian matrices on H_1 and H_2 is presented. From this construction we have shown that a state is separable if and only if the separability indicator is positive. In principle one can always get a Hermitian tensor product decomposition of a density matrix by using a basic set of Hermitian matrices. Our approach gives a decomposition with minimum terms (the number of the terms depends on the rank of \hat{A}_{22}), similar to the Schmidt decomposition for bipartite pure states. In example (30) we see that the 8×8 density matrix ρ_b has only 4 terms in the tensor product decomposition.

In [27] an entanglement measure called robustness is introduced. For a mixed state ρ and a separable state ρ_s , the robustness of ρ relative to ρ_s , $R(\rho||\rho_s)$, is the minimal $s \geq 0$ for which the density matrix $(\rho + s\rho_s)/(1 + s)$ is separable, i.e. the minimal amount of mixing with locally prepared states which washes out all entanglement. In particular, the random robustness of ρ is the one when ρ_s is taken to be the (separable) identity matrix. In this case ρ has the form $\rho = (1 + t)\rho_s^+ - tI_m \otimes I_n/mn$, where ρ_s^+ is separable. ρ is separable if and if the minimum of t is zero. Therefore the separability indicator appeared from our matrix decompositions is basically the minus of the random robustness, up to a normalization. Another interesting separable approximations of density matrices was presented in [28]. This method, so called best separable approximations, was based on subtracting projections on product vectors from a given density matrix in such a way that the remainder remained positively defined. In stead expressing a density matrix as the sum of a separable part and the identity part, this approximation gives rise to a sum of a separable part and an entangled part from which no more projections on product vectors can be subtracted.

The results can be generalized to multipartite states. Let's consider a general l -partite mixed state $\rho_{1,2,\dots,l}$ on space $H_1 \otimes H_2 \otimes \dots \otimes H_l$. We can first consider $\rho_{1,2,\dots,l}$ as a bipartite state on space H_1 and $H_2 \otimes \dots \otimes H_l$. By using Theorem 2 we can find the tensor decomposition $\rho_{1,2,\dots,l} = \sum_{i=1}^{r_1} B_i^1 \otimes B_i^{23\dots l}$, where B_i^1 and $B_i^{23\dots l}$ are Hermitian matrices on H_1 and $H_2 \otimes \dots \otimes H_l$ respectively. The matrices $B_i^{23\dots l}$ can be again decomposed as $B_i^{23\dots l} = \sum_{j=1}^{r_2} B_{ij}^2 \otimes B_{ij}^{3\dots l}$, $\forall i$, with B_{ij}^2 and $B_{ij}^{3\dots l}$ being Hermitian matrices on H_2 and $H_3 \otimes \dots \otimes H_l$ respectively. In doing so at last we have the Hermitian tensor product decomposition of the form, $\rho_{1,2,\dots,l} = \sum_{i=1}^r B_i^1 \otimes B_i^2 \otimes \dots \otimes B_i^l$, where B_i^k are Hermitian matrices on H_k . New decompositions can be obtained, $\rho_{1,2,\dots,l} = \sum_{i=1}^{r'} B_i'^1 \otimes B_i'^2 \otimes \dots \otimes B_i'^l$, where $B_i'^k = \sum_{j=1}^r E_{ij}^k B_j^k$, $k = 1, \dots, l$, $E^k = (E_{ij}^k)$ are the real matrices satisfying $\sum_{j=1}^{r'} E_{i_1 j}^1 E_{i_2 j}^2 \dots E_{i_l j}^l = \delta_{i_1 i_2} \delta_{i_2 i_3} \dots \delta_{i_{l-1} i_l}$.

For any given decompositions, in terms of the protocol (31), one has $\rho_{1,2,\dots,l} = \sum_{i=1}^{r'} B_i'^1 \otimes B_i'^2 \otimes \dots \otimes B_i'^l + q Id_1 \otimes Id_2 \otimes \dots \otimes Id_l$, where Id_i is the identity matrix on H_i , $(B_i'^1, B_i'^2, \dots,$

B_i^l) are Hermitian matrices such that $m(B_i^k) = 0$, or part of them (but not all) are identity matrices. The separability indicator $S(\rho_{1,2,\dots,l})$ is the maximal value of the parameter q for all possible positive Hermitian tensor product decompositions. If the parameter $S(\rho_{1,2,\dots,l}) \geq 0$, the state $\rho_{1,2,\dots,l}$ is separable, otherwise it is entangled.

Acknowledgments S.M. Fei gratefully acknowledges the warm hospitality of Dept. Math., NCSU and the support provided by American Mathematical Society. Jing greatly acknowledges the support from the NSA and Alexander von Humboldt foundation.

References

- [1] J. Preskill, The Theory of Quantum Information and Quantum Computation, California Inst. of Tech., 2000, <http://www.theory.caltech.edu/people/preskill/ph229/>.
- [2] M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, Cambridge, 2000.
- [3] D. Bouwmeester, A. Ekert and A. Zeilinger (Eds.), The Physics of Quantum Information: Quantum Cryptography, Quantum Teleportation and Quantum Computation, Springer, New York, 2000.
- [4] M. Lewenstein, D. Bruss, J.I. Cirac, B. Kraus, M. Kus, J. Samsonowicz, A. Sanpera and R. Tarrach, J. Mod. Opt. **47**, 2841 (2000).
- [5] B.M. Terhal, Theor. Comput. Sci. **287**, 313 (2002).
- [6] M. Horodecki, P. Horodecki and R. Horodecki, Springer Tracts in Mod. Phys. **173**, 151 (2001).
- [7] J.S. Bell, Physics (N.Y.) **1**, 195 (1964).
- [8] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
- [9] M. Horodecki, P. Horodecki and R. Horodecki, Phys. Lett. A **223**, 1 (1996).
- [10] M. Horodecki and P. Horodecki, Phys. Rev. A **59**, 4206 (1999).
- [11] N.J. Cerf, C. Adami and R.M. Gingrich, Phys. Rev. A **60**, 898 (1999).
- [12] M.A. Nielsen and J. Kempe, Phys. Rev. Lett. **86**, 5184 (2001).
- [13] B. Terhal, Phys. Lett. A **271**, 319 (2000).
- [14] M. Lewenstein, B. Kraus, J.I. Cirac and P. Horodecki, Phys. Rev. A **62**, 052310 (2000).
- [15] O. Rudolph, Physical Review A **67**, 032312 (2003).
- [16] K. Chen and L.A. Wu, Quant. Inf. Comput. **3**, 193 (2003).
- [17] K. Chen and L.A. Wu, Phys. Lett. A **306**, 14 (2002).

- [18] S. Albeverio, K. Chen and S.M. Fei, Phys. Rev. A **68**, 062313 (2003).
- [19] P. Horodecki, M. Lewenstein, G. Vidal and I. Cirac, Phys. Rev. A **62**, 032310 (2000).
- [20] S. Albeverio, S.M. Fei and D. Goswami, Phys. Lett. A **286**, 91 (2001).
- [21] S.M. Fei, X.H. Gao, X.H. Wang, Z.X. Wang and K. Wu, Phys. Lett. A **300**, 555 (2002).
- [22] G.H. Golub, C.F. von Loan, *Matrix Computation*, The Johns Hopkins University Press, 1989.
- [23] C.F. Van Loan and N.P. Pitsianis, in: Linear Algebra for Large Scale and Real Time Applications, M.S. Moonen and G.H. Golub (Eds.), Kluwer Publications, 1993, pp. 293–314.
- [24] N.P. Pitsianis, Ph.D. thesis, *The Kronecker Product in Approximation and Fast Transform Generation*, Cornell University, New York (1997).
- [25] R.F. Werner, Phys. Rev. A **40**, 4277 (1989).
- [26] P. Horodecki, Phys. Lett. A **232**, 333 (1997).
- [27] G. Vidal and R. Tarrach, Phys.Rev. A **59**, 141(1999).
- [28] S. Karnas and M. Lewenstein, J. Phys. A **34**, 6919(2001).